

New results on the cp rank and related properties of co(mpletely)positive matrices

Naomi Shaked-Monderer¹

Emek Yezreel College, Israel

Abraham Berman¹

Dept. of Mathematics, Technion, Haifa, Israel

Immanuel M. Bomze

ISOR, University of Vienna, Austria

Florian Jarre

Mathem. Institut, University of Düsseldorf, Germany

Werner Schachinger

ISOR, University of Vienna, Austria

Abstract

Copositive and completely positive matrices play an increasingly important role in Applied Mathematics, namely as a key concept for approximating NP-hard optimization problems. The cone of copositive matrices of a given order and the cone of completely positive matrices of the same order are dual to each other with respect to the standard scalar product on the space of symmetric matrices. This paper establishes some new relations between orthogonal pairs of such matrices lying on the boundary of either cone. As a consequence, we can establish an improvement on the upper bound of the cp-rank of completely positive matrices of general order, and a further improvement for such matrices of order six.

Key words: copositive optimization, completely positive matrices, cp-rank, nonnegative factorization.

AMS classification: 15B48, 90C25, 15A23

May 6, 2013

¹The work of Abraham Berman and Naomi Shaked-Monderer was supported by grant no. G-18-304.2/2011 by the German-Israeli Foundation for Scientific Research and Development (GIF).

1 Introduction

In this article we consider completely positive matrices and their cp-rank, as well as copositive matrices. An $n \times n$ matrix M is said to be *completely positive* if there exists a nonnegative (not necessarily square) matrix V such that $M = VV^\top$. An $n \times n$ matrix A is said to be *copositive* if $\mathbf{x}^\top A \mathbf{x} \geq 0$ for every nonnegative vector $\mathbf{x} \in \mathbb{R}_+^n$. The completely positive matrices of order n form a cone, \mathcal{C}_n^* , dual to the cone of copositive matrices of that order, \mathcal{C}_n . Both cones are central in the rapidly evolving field of *copositive optimization* which links discrete and continuous optimization, and has numerous real-world applications. For recent surveys and structured bibliographies, we refer to [4, 5, 6, 11], and for a fundamental text book to [3].

A main motivation for this paper was the study of cp-rank: A given completely positive matrix M always has many factorizations $M = VV^\top$, where V is a nonnegative matrix, and the *cp-rank* of M , $\text{cpr } M$, is the minimum number of columns in such a nonnegative factor V (for completeness, we define $\text{cpr } M = 0$ if M is a square zero matrix and $\text{cpr } M = \infty$ if M is not completely positive). Determining the maximum possible cp-rank of $n \times n$ completely positive matrices,

$$p_n := \max \{ \text{cpr } M : M \text{ is a completely positive } n \times n \text{ matrix} \},$$

is still an open problem for large n (up to now, for $n \geq 6$; only recently $p_5 = 6$ has been established [18]). It is known [3, Theorem 3.3] that

$$p_n = n \quad \text{if } n \leq 4. \tag{1}$$

For $n \in \{2, 3\}$, there exist simple proofs of (1), but already for $n = 4$, the argument is quite involved [3]. For $n \geq 5$, it is known that

$$d_n := \left\lfloor \frac{n^2}{4} \right\rfloor \leq p_n \leq \binom{n+1}{2} - 1, \tag{2}$$

but whether the lower bound d_n is in fact equal to p_n is still unknown for large n . This is the famous Drew-Johnson-Loewy (DJL) conjecture [10]. The above upper bound on p_n on the right-hand side follows, for example, from the so-called Barioli-Berman [1] bound: Let

$$b_r := \max \{ \text{cpr } M : M \text{ is a completely positive matrix with rank } M = r \},$$

then for $r \geq 3$

$$b_r = \binom{r+1}{2} - 1. \tag{3}$$

Some evidence in support of the DJL conjecture is found in [10, 9, 2, 16], see also [3, Section 3.3]. The DJL conjecture has recently been proved for $n = 5$ [18], but the cp-rank problem is still not fully resolved. Not only is it

not known whether the DJL conjecture holds, but the best upper bound on p_n for $n \geq 6$ remained, for over a decade, b_n . Two main results of this paper are a reduction of the upper bound on p_n in the bracket (2) for general n and a further reduction in case of $n = 6$. To obtain these results, we use [18, Thm.3.4], which guarantees that p_n is attained (also) at a nonsingular matrix on the boundary of the cone of \mathcal{C}_n^* . We also complement this result here by studying, for every possible cp-rank $1 \leq k \leq p_n$, where in \mathcal{C}_n^* is cp-rank k attained.

Each matrix on the boundary of the cone \mathcal{C}_n^* is orthogonal to a matrix on the boundary of the cone \mathcal{C}_n (in fact, to a matrix generating an extreme ray of that cone). Thus to improve the bound on p_n we consider pairs of matrices, $M \in \mathcal{C}_n^*$ and $A \in \mathcal{C}_n$, that are orthogonal to each other in the standard scalar product of matrices. This leads also to some results that are not directly related to the cp-rank problem, and are of interest in their own right.

The paper is organized as follows: after introducing basic concepts and terminology, we show, in Section 2, some important orthogonality and diagonal dominance results. Section 3 is devoted to the study of extreme copositive matrices of low rank, while Section 4 deals with genericity of the property of having a fixed cp-rank within the completely positive cone. Section 5 presents improvements of upper bounds on the cp-rank for matrices of general order, and a further tightening of this bound for order six is put forward in the final Section 6.

Some notation and terminology: let \mathbf{e}_i be the i th column vector of the $n \times n$ identity matrix I_n . The nonnegative orthant is denoted by \mathbb{R}_+^n . For a vector $\mathbf{x} \in \mathbb{R}_+^n$, the *support* of \mathbf{x} is denoted by $\sigma(\mathbf{x})$, i.e.,

$$\sigma(\mathbf{x}) = \{i : x_i > 0\}.$$

The set of nonnegative $n \times p$ matrices is denoted by $\mathbb{R}_+^{n \times p}$. A matrix $A \in \mathbb{R}_+^{n \times p}$ is called *positive* if $\min_{i,j} A_{ij} > 0$. (Note that a completely positive matrix is not necessarily positive, since it may have zero entries.) A matrix $A \in \mathbb{R}^{n \times n}$ is *diagonally dominant* if $|A_{ii}| \geq \sum_{j \neq i} |A_{ij}|$ for every $1 \leq i \leq n$, and is *strictly diagonally dominant* if all these n inequalities are strict. For two square matrices A, B we denote

$$A \oplus B = \begin{bmatrix} A & O \\ O^\top & B \end{bmatrix},$$

where O is a suitable (possibly rectangular) zero matrix.

By \mathcal{S}_n we denote the space of real symmetric $n \times n$ matrices, and by \mathcal{P}_n the cone of symmetric psd matrices, $\mathcal{P}_n = \{X \in \mathcal{S}_n : X \succeq 0\}$. The cone of nonnegative matrices in \mathcal{S}_n is denoted by \mathcal{N}_n , i.e., $\mathcal{N}_n = \mathcal{S}_n \cap \mathbb{R}_+^{n \times n}$. The scalar product of two matrices U, V of same order is

$\langle U, V \rangle := \text{trace}(U^\top V) = \sum_{i,j} U_{ij} V_{ij}$. If $V = [\mathbf{v}_1, \dots, \mathbf{v}_p] \in \mathbb{R}_+^{n \times p}$, then the factorization $M = VV^\top$ is equivalent to $M = \sum_{i=1}^p \mathbf{v}_i \mathbf{v}_i^\top$. We refer to this sum as a *cp decomposition*. When $p = \text{cpr } M$ we say that the cp decomposition is *minimal* (the cp factorization is minimal).

By K° we denote the *relative interior* of a convex set K , ∂K is the *boundary* of that set. For a convex cone K , $\text{ext } K$ denotes the set of all elements in K who generate extreme rays of K .

Both the copositive cone \mathcal{C}_n and the completely positive cone \mathcal{C}_n^* , are pointed closed convex cones with nonempty interior. As mentioned above, the copositive cone \mathcal{C}_n and, in particular, its extremal rays, are important for the study of the cp-rank as any matrix on the boundary $\partial \mathcal{C}_n^*$ of \mathcal{C}_n^* is orthogonal to an extremal ray of \mathcal{C}_n . However, characterization of the extremal rays of \mathcal{C}_n for $n > 5$ is itself a major open problem in the study of \mathcal{C}_n . The explicit characterization of extremal rays of \mathcal{C}_5 was completed by Hildebrand [14] only recently, and this work was essential for the arguments in [18]. One extremal ray of \mathcal{C}_5 is generated by the so-called *Horn matrix*

$$H = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix},$$

which historically was the first copositive matrix detected outside of $\mathcal{P}_n + \mathcal{N}_n$ (here $n = 5$) [7]; attribution to Alfred Horn can be found in [13]. In the sequel, a matrix A is said to be *in the orbit* of a matrix B if $A = DP^\top BPD$, where D is a positive-definite diagonal matrix and P a permutation matrix. The *Horn orbit* consists of all matrices in the orbit of H ; obviously, each matrix in the Horn orbit also generates an extremal ray of \mathcal{C}_5 . Finally, we address any extremal matrix in \mathcal{C}_5 which is neither in the Horn orbit nor in $\mathcal{P}_5 \cup \mathcal{N}_5$ as a *Hildebrand matrix*; see description in [18, Thm.4.2].

2 Orthogonality and diagonal dominance results

In this section we consider copositive and completely positive matrices which are orthogonal to each other. The following theorem will be used in this section to point out a property of matrices on the boundary of the copositive cone, and also later to reduce the upper bound for p_n .

Theorem 2.1 *Let $M \in \mathcal{C}_n^*$ be orthogonal to $A \in \mathcal{C}_n$, and let $M = \sum_{j=1}^p \mathbf{x}_j \mathbf{x}_j^\top$ be any cp decomposition of M . Then*

- (a) *For every $1 \leq i \leq n$ the i -th column of M is orthogonal to the i -th column of A .*

(b) If $i \in \sigma(\mathbf{x}_j)$ for every $1 \leq j \leq p$, then the i -th column of A is in the nullspace of M .

Proof. The scalar product of the ℓ -th column of M and the i -th column of A is

$$\mathbf{e}_\ell^\top M \mathbf{A} \mathbf{e}_i = \sum_{j=1}^p \mathbf{e}_\ell^\top \mathbf{x}_j \mathbf{x}_j^\top \mathbf{A} \mathbf{e}_i = \sum_{j: \ell \in \sigma(\mathbf{x}_j)} \left(\mathbf{e}_\ell^\top \mathbf{x}_j \right) \left(\mathbf{x}_j^\top \mathbf{A} \mathbf{e}_i \right). \quad (4)$$

(a) If $\ell = i$, the right-hand side in (4) is

$$\sum_{j: i \in \sigma(\mathbf{x}_j)} \left(\mathbf{e}_i^\top \mathbf{x}_j \right) [\mathbf{A} \mathbf{x}_j]_i.$$

Since each \mathbf{x}_j is in \mathbb{R}_+^n and satisfies $\mathbf{x}_j^\top \mathbf{A} \mathbf{x}_j = 0$ we have $[\mathbf{A} \mathbf{x}_j]_k = 0$ for all $k \in \sigma(\mathbf{x}_j)$ [18, Rem.3.2, (3.1)]. In particular $[\mathbf{A} \mathbf{x}_j]_i = 0$ for all j 's in the sum above. Hence $\mathbf{e}_i^\top M \mathbf{A} \mathbf{e}_i = 0$.

(b) Let $\mathbf{z} = \mathbf{A} \mathbf{e}_i$. Suppose $i \in \sigma(\mathbf{x}_j)$ for all $j \in \{1, \dots, p\}$, then as above $[\mathbf{A} \mathbf{x}_j]_i = 0$ for every j , and thus by (4)

$$[M \mathbf{z}]_\ell = \mathbf{e}_\ell^\top M \mathbf{A} \mathbf{e}_i = \sum_{j=1}^p \left(\mathbf{e}_\ell^\top \mathbf{x}_j \right) \left(\mathbf{x}_j^\top \mathbf{A} \mathbf{e}_i \right) = \sum_{j=1}^p \left(\mathbf{e}_\ell^\top \mathbf{x}_j \right) [\mathbf{A} \mathbf{x}_j]_i = 0$$

for every $\ell \in \{1, \dots, n\}$. □

Before we proceed, we note an interesting implication about *copositive* matrices on the boundary $\partial \mathcal{C}_n$. It is well known, and obvious by a Gershgorin-type argument, that singular matrices (e.g. those on $\partial \mathcal{P}_n$) cannot be strictly diagonally dominant. For matrices on $\partial \mathcal{C}_n$ we show that some form of “anti-diagonal dominance” can be established:

Corollary 2.1 *Let $A \in \partial \mathcal{C}_n$. If $A \perp M \in \mathcal{C}_n^*$ and M has no zero rows, then A is in the orbit of some $\bar{A} \in \partial \mathcal{C}_n$ which satisfies*

$$\bar{A}_{ii} \leq \sum_{j \neq i} |\bar{A}_{ij}| \quad \text{for all } i.$$

Proof. If $A = O$, this is trivial. Else, for $A \in \partial \mathcal{C}_n \setminus \{O\}$, we select $M \in \mathcal{C}_n^* \cap A^\perp \setminus \{O\}$ and choose $\mathbf{u}_i \in \mathbb{R}_+^p$ where $p = \text{cpr } M$, $1 \leq i \leq n$, such that $M_{ij} = \mathbf{u}_i^\top \mathbf{u}_j$ (in other words, M is the Gram matrix of $\mathbf{u}_1, \dots, \mathbf{u}_n$). Next we select i so that $\|\mathbf{u}_i\| \geq \|\mathbf{u}_j\|$ for all j . Then, since $M \neq O$, we have $\|\mathbf{u}_i\| > 0$ and

$$\sum_{j \neq i} A_{ij} \mathbf{u}_i^\top \mathbf{u}_j = (\mathbf{A} \mathbf{e}_i)^\top (M \mathbf{e}_i) - A_{ii} \|\mathbf{u}_i\|^2 = -A_{ii} \|\mathbf{u}_i\|^2,$$

by Theorem 2.1(a). Passing to absolute values and applying Cauchy-Schwarz as well as the triangle inequality, we get

$$A_{ii} \leq \sum_{j \neq i} \frac{\|\mathbf{u}_j\|}{\|\mathbf{u}_i\|} |A_{ij}| \leq \sum_{j \neq i} |A_{ij}|.$$

Scaling M by a positive-definite diagonal matrix D so that $\bar{M} = DMD$ has $\text{diag } \bar{M} = \mathbf{e}$, we get that $\bar{A} = D^{-1}AD^{-1}$ satisfies $\bar{A} \perp \bar{M}$, so that the above inequality holds for all i , if we replace A with \bar{A} . \square

According to a result by Kaykobad [15], any symmetric diagonally dominant matrix in \mathcal{N}_n is already completely positive. Triggered by above, we could ask whether indeed these matrices are in the interior of \mathcal{C}_n^* . The answer is negative, a certificate being I_n : matrices in the interior of \mathcal{C}_n^* are necessarily positive. In general, being nonsingular and positive is not a sufficient condition for an $n \times n$ completely positive matrix to be in $[\mathcal{C}_n^*]^\circ$. However, we can prove the following

Theorem 2.2 *Let M be an $n \times n$ symmetric matrix, $n \geq 3$. If M is diagonally dominant and positive, then $M \in [\mathcal{C}_n^*]^\circ$.*

Proof. Let $\mathbf{e} = [1, \dots, 1]^\top \in \mathbb{R}^n$, $J_n = \mathbf{e}\mathbf{e}^\top$ denote the all ones $n \times n$ matrix, and let $\mu := \min_{i,j} M_{ij} > 0$. Consider $M' := M - \mu J_n$. Since $n \geq 3$, $M' \in \mathcal{N}_n$ is strictly diagonally dominant and therefore completely positive and nonsingular. So we can put $M = VV^\top$ where $\mathbf{v}_1 = \sqrt{\mu}\mathbf{e}$, and the remaining \mathbf{v}_i come from the cp factorization of M' . By Dickinson's characterization [8] of $[\mathcal{C}_n^*]^\circ$, the assertion is proved. \square

Note that for $n = 2$ there exist diagonally dominant matrices that are not in $[\mathcal{C}_2^*]^\circ$, e.g., J_2 , which is singular, and therefore on $\partial\mathcal{C}_2^*$.

3 Extreme copositive matrices of low rank

If $A \in \text{ext } \mathcal{C}_n \cap \mathcal{N}_n$, then there is at most one positive entry on or above the diagonal. If this entry is on the diagonal, we have $\text{rank } A = 1$ and $A \in \mathcal{P}_n$. If the positive entry is off the diagonal, then A is in the orbit of the matrix $E_{12} = \mathbf{e}_1\mathbf{e}_2^\top + \mathbf{e}_2\mathbf{e}_1^\top$, and hence is of rank two. Next we will sharpen these assertions, basically dropping the nonnegativity assumption on A . We will need the following auxiliary result, on the role of zero entries on the diagonal of an extreme copositive matrix:

Lemma 3.1 *Suppose that $A \in \text{ext } \mathcal{C}_n \setminus \mathcal{N}_n$ can be decomposed as*

$$A = \begin{bmatrix} S & R \\ R^\top & Q \end{bmatrix}, \quad \text{with } S \in \mathcal{S}_k \text{ and } \text{diag } Q = \mathbf{o} \in \mathbb{R}^{n-k}, k \geq 1.$$

Then R and Q are zero matrices (of suitable orders) and $S \in \text{ext } \mathcal{C}_k \setminus \{O\}$.

Proof. Since $\text{diag } Q = \mathbf{o}$ and $A \in \mathcal{C}_n$, we deduce $Q \in \mathbb{R}_+^{(n-k) \times (n-k)}$ and $R \in \mathbb{R}_+^{k \times (n-k)}$. Further, since $A \notin \mathcal{N}_n$, $S \in \mathbb{R}^{k \times k}$ has at least one negative element. Thus $k \geq 1$ and $S \neq O$. We conclude that

$$A = \begin{bmatrix} S & O \\ O & O \end{bmatrix} + \begin{bmatrix} O & R \\ R^\top & Q \end{bmatrix},$$

where the rightmost matrix has no negative entries and therefore is copositive. As $S \neq O$, extremality of A implies that both Q and R have to be zero matrices, and $A = S \oplus O$ as well as extremality of S in \mathcal{C}_k follows. \square

We can now prove:

Theorem 3.1 *Let $A \in \text{ext } \mathcal{C}_n$. Then*

- (a) *rank $A = 1$ if and only if A is positive-semidefinite.*
- (b) *rank $A = 2$ if and only if A is in the orbit of $E_{12} = \mathbf{e}_1 \mathbf{e}_2^\top + \mathbf{e}_2 \mathbf{e}_1^\top$.*

Proof. The if parts are obvious. For the only if:

- (a) If rank $A = 1$ then, since A is symmetric, $A = \pm \mathbf{x} \mathbf{x}^\top$ for some $\mathbf{x} \in \mathbb{R}^n$. Since the diagonal entries of A are nonnegative, $A = \mathbf{x} \mathbf{x}^\top$.
- (b) Suppose rank $A = 2$; if $A \in \mathcal{N}_n$, then the result follows directly. So suppose A has a negative entry. By extremality $A \notin \mathcal{P}_n$. Hence A must be indefinite, i.e. of the form $A = \mathbf{u} \mathbf{u}^\top - \mathbf{v} \mathbf{v}^\top = \mathbf{x} \mathbf{y}^\top + \mathbf{y} \mathbf{x}^\top$ (take, e.g., $\mathbf{x} = \frac{1}{2}(\mathbf{u} + \mathbf{v})$ and $\mathbf{y} = \mathbf{u} - \mathbf{v}$). For any $\mathbf{z} \in \mathbb{R}_+^n$ we have

$$0 \leq \mathbf{z}^\top A \mathbf{z} = 2(\mathbf{x}^\top \mathbf{z})(\mathbf{y}^\top \mathbf{z}),$$

in particular $x_i y_i \geq 0$ for all i . Put $\tau := \{i : x_i y_i \neq 0\}$. Then $x_i y_i > 0$ for all $i \in \tau$. By permuting rows and columns if necessary, we may assume that $\tau = \{1, \dots, k\}$, and A can be decomposed as in Lemma 3.1, yielding $A = S \oplus O$. So we may without loss of generality assume that $x_i y_i > 0$ holds for all i , by investigating S instead of A . By diagonal scaling we may now further assume that $x_i y_i = 1$ for all i . Now, if both $\mathbf{x}, \mathbf{y} \in \mathbb{R}_+^n$ or both $-\mathbf{x}, -\mathbf{y} \in \mathbb{R}_+^n$, we again would arrive at $A \in \mathcal{N}_n$. So we are done if we reduce the assumption $x_i > 0 > x_j$ *ad absurdum*. To this end, consider the 2×2 block corresponding to these two indices $\{i, j\}$, putting $t = \frac{x_i}{x_j} < 0$:

$$\begin{bmatrix} 2x_i y_i & x_i y_j + y_i x_j \\ x_i y_j + y_i x_j & 2x_j y_j \end{bmatrix} = \begin{bmatrix} 2 & t + \frac{1}{t} \\ t + \frac{1}{t} & 2 \end{bmatrix} \in \mathcal{C}_2.$$

Copositivity of this 2×2 matrix is equivalent to the condition $t + \frac{1}{t} \geq -2$, which upon multiplication with $t < 0$ amounts to $(t + 1)^2 \leq 0$ or $t = -1$. So all positive entries of \mathbf{x} are equal, say α , and all negative entries of \mathbf{x} equal $-\alpha$. Hence \mathbf{y} is a multiple of \mathbf{x} and $\text{rank } A = 1 < 2$, a contradiction.

□

Remark 3.1 *Theorem 3.1 implies that for $n \leq 4$ each matrix in $\text{ext } \mathcal{C}_n \setminus \{O\}$ has rank 1 or 2. The characterization of the extreme copositive 5×5 matrices implies that each matrix in $\text{ext } \mathcal{C}_5 \setminus \{O\}$ has rank 1, 2, or 5 [14]. What are the possible ranks of matrices in $\text{ext } \mathcal{C}_n$, $n \geq 6$? Note that if there exists $A \in \text{ext } \mathcal{C}_n$ of rank k , then there exist also matrices in $\text{ext } \mathcal{C}_{n+1}$ of rank k ($A \oplus 0$, to name one).*

We proceed with an immediate consequence for positive and nonsingular matrices $M \in \partial \mathcal{C}_n^*$:

Corollary 3.1 *If $M \in \partial \mathcal{C}_n^* \setminus (\partial \mathcal{P}_n \cup \partial \mathcal{N}_n)$, then any $A \in \text{ext } \mathcal{C}_n \cap M^\perp \setminus \{O\}$ satisfies $\text{rank } A \geq 3$. Moreover, no principal submatrix S of A can be in the orbit of E_{12} .*

Proof. Because M is assumed to be positive, we know $A \notin \mathcal{N}_n$; similarly, since M is nonsingular, we conclude $A \notin \mathcal{P}_n$. Therefore Theorem 3.1 implies $\text{rank } A \geq 3$. Next suppose a principal submatrix $S \neq O$ of A were in the orbit of E_{12} and thus has $\text{diag } S = \mathbf{o}$. Then A can be decomposed into

$$A = \begin{bmatrix} S & O \\ O & O \end{bmatrix} + \begin{bmatrix} O & R \\ R^\top & Q \end{bmatrix},$$

where R has no negative entries and Q is copositive. Hence the rightmost matrix is copositive, and (by extremality of A and $S \neq O$) therefore must be the zero matrix. It follows $\text{rank } A = \text{rank } S \oplus O = \text{rank } S = 2$, but then Theorem 3.1(b) yields the contradiction $A \in \partial \mathcal{N}_n$. □

4 Genericity of matrices of fixed cp rank and order

We now turn to the study of the cp-rank of matrices in \mathcal{C}_n^* . In this section we consider the question whether or not having a certain cp rank is robust within all cp matrices of order n or not.

First we observe that every possible cp-rank is attained at some matrix on the boundary:

Proposition 4.1 *For every $1 \leq k \leq p_n$ there exists a matrix $M_k \in \partial \mathcal{C}_n^*$ such that $\text{cpr } M_k = k$.*

Proof. By [18, Thm.3.4] there exists a matrix $M \in \partial \mathcal{C}_n^*$ with $\text{cpr } M = p_n$. Let $M = \sum_{j=1}^{p_n} \mathbf{v}_j \mathbf{v}_j^\top$ be a minimal cp-decomposition of M , and let $M_k = \sum_{j=1}^k \mathbf{v}_j \mathbf{v}_j^\top$. Then $\text{cpr } M_k \leq k$, and strict inequality is impossible, because it would contradict the minimality of the cp-decomposition of M . That is, $\text{cpr } M_k = k$. Since M is on the boundary of \mathcal{C}_n^* , there exists $A \in \partial \mathcal{C}_n \setminus \{O\}$ such that M is orthogonal to A . Then $\mathbf{v}_j \mathbf{v}_j^\top \perp A$ for every j , and thus $M_k \perp A$, and therefore $M_k \in \partial \mathcal{C}_n^*$. \square

However, it is interesting to find out whether there are also interior matrices having a prescribed cp-rank, and whether this property is robust. For this purpose, we denote the set of completely positive matrices of order n with cp-rank exactly equal to k by

$$\mathcal{C}_{n,k}^* = \{M \in \mathcal{C}_n^* : \text{cpr } M = k\}.$$

The extreme case $k = p_n$ is easy: as shown in [18, Cor.2.5], the set \mathcal{C}_{n,p_n}^* contains an open set, and thus, $[\mathcal{C}_{n,p_n}^*]^\circ \neq \emptyset$. To prove this for all other k , we need a result which may also be of independent interest. Beforehand note that every $M \in [\mathcal{C}_{n,p_n}^*]^\circ$ has a factorization $M = VV^\top$ where $V \geq 0$ has p_n columns, and by the Dür and Still characterization of $[\mathcal{C}_n^*]^\circ$ [12] it is easy to deduce that there exists a factorization $M = WW^\top$ where W is positive (and has rank n). However, this does not necessarily imply that there is a factorization $M = VV^\top$ where $V \geq 0$ has p_n columns and all of these columns are positive.

Proposition 4.2 *There is always a matrix $M \in [\mathcal{C}_{n,p_n}^*]^\circ$ such that there exists a positive $n \times p_n$ matrix V with $M = VV^\top$.*

Proof. Let M_0 be some matrix in the interior of \mathcal{C}_{n,p_n}^* . As in [18], let $\mathbf{v} \in [\mathbb{R}_+^n]^\circ$ be its Perron-Frobenius eigenvector to the eigenvalue $\lambda > 0$. If $M_0 = V_0 V_0^\top$ where V_0 is a nonnegative $n \times p_n$ -matrix, then no column $V_0 \mathbf{e}_i$ of V_0 is zero. Therefore $(V_0^\top \mathbf{v})_i = \mathbf{v}^\top V_0 \mathbf{e}_i > 0$ for all i , in other words, $\tilde{\mathbf{x}} := V_0^\top \mathbf{v} \in [\mathbb{R}_+^{p_n}]^\circ$. From $\lambda \mathbf{v} = M_0 \mathbf{v} = V_0 V_0^\top \mathbf{v} = V_0 \tilde{\mathbf{x}}$ it follows that $\mathbf{x} := \tilde{\mathbf{x}}/\lambda$ is a positive vector with $\mathbf{v} = V_0 \mathbf{x}$. For small $\varepsilon > 0$ it follows from the choice of M_0 that $M = M_0 + \varepsilon \mathbf{v} \mathbf{v}^\top$ also has $\text{cpr } (M) = p_n$. Now

$$M = M_0 + \varepsilon \mathbf{v} \mathbf{v}^\top = V_0 V_0^\top + (V_0 \mathbf{x}) \varepsilon (V_0 \mathbf{x})^\top = V_0 (I_n + \varepsilon \mathbf{x} \mathbf{x}^\top) V_0^\top. \quad (5)$$

For $\delta = (\sqrt{1 + \varepsilon \mathbf{x}^\top \mathbf{x}} - 1)/\|\mathbf{x}\| > 0$, define $C = I_n + \delta \mathbf{x} \mathbf{x}^\top$. Then $C^2 = I_n + \varepsilon \mathbf{x} \mathbf{x}^\top$ and $V = V_0 C = V_0 + \delta (V_0 \mathbf{x}) \mathbf{x}^\top$ is positive (as before, $V_0 \mathbf{x} \in [\mathbb{R}_+^{p_n}]^\circ$). By (5) we obtain $VV^\top = V_0 C^2 V_0^\top = M$. \square

Theorem 4.1

$$[\mathcal{C}_{n,k}^*]^\circ \neq \emptyset \iff n \leq k \leq p_n.$$

Proof. For $k < n$ it follows from $\text{cpr}(M) \geq \text{rank}(M)$ that $\mathcal{C}_{n,k}^*$ is contained in the set of matrices with rank at most k and thus its interior is empty. We now show that $[\mathcal{C}_{n,k}^*]^\circ \neq \emptyset$ if $n \leq k \leq p_n$. To this end, Proposition 4.2 ensures we can select a matrix $M = VV^\top \in [\mathcal{C}_{n,p_n}^*]^\circ$ with a positive $n \times p_n$ matrix $V = [\mathbf{v}_1, \dots, \mathbf{v}_{p_n}]$. As $M \in [\mathcal{C}_n^*]^\circ \subset \mathcal{P}_n^\circ$, we have $\text{rank } V = n$ and without loss of generality, let the first n columns $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ of V be linearly independent. Now, let any k with $n \leq k \leq p_n$ be given and consider the matrix

$$\overline{M} := \sum_{j=1}^k \mathbf{v}_j \mathbf{v}_j^\top.$$

Obviously $\text{cpr } \overline{M} \leq k$. On the other hand, $\text{cpr } \overline{M} < k$ would contradict the minimality of the factorization $M = VV^\top$, so $\text{cpr } \overline{M} = k$. Let $\overline{V} := [\mathbf{v}_1, \dots, \mathbf{v}_n]$ and $\tilde{V} := [\mathbf{v}_{n+1}, \dots, \mathbf{v}_k]$. Then \overline{V} is positive and non-singular square, so by [12, Thm.2.3], we have $\overline{M} = \overline{V}\overline{V}^\top + \tilde{V}\tilde{V}^\top \in [\mathcal{C}_n^*]^\circ$. Next consider the singular value decomposition of $\overline{V} = U_1 \Sigma U_2$ with suitable orthonormal $n \times n$ matrices U_1 and U_2 and a positive-definite diagonal $n \times n$ matrix Σ . Let $U_2^\top \mathcal{S}_n U_1^\top$ be the set of all matrices of order n which result from premultiplying a symmetric matrix Z by U_2^\top and postmultiplying it by U_1^\top . Consider the map $\mathcal{F} : U_2^\top \mathcal{S}_n U_1^\top \rightarrow \mathcal{S}_n$ defined by $\mathcal{F}(\Delta V) := (\overline{V} + \Delta V)(\overline{V} + \Delta V)^\top$. The derivative of \mathcal{F} at $\Delta V = 0$ is given by the Lyapunov operator

$$\mathcal{L}_{\overline{V}} : U_2^\top \mathcal{S}_n U_1^\top \rightarrow \mathcal{S}_n \quad \text{with} \quad \mathcal{L}_{\overline{V}}(\Delta V) = (\Delta V)\overline{V}^\top + \overline{V}(\Delta V)^\top.$$

Given a symmetric right hand side R , solving $\mathcal{L}_{\overline{V}}(U_2^\top Z U_1^\top) = R$ for a symmetric matrix Z is equivalent to

$$\begin{aligned} U_2^\top Z U_1^\top U_1 \Sigma U_2 + U_2^\top \Sigma U_1^\top U_1 Z U_2 &= R \\ \iff Z \Sigma + \Sigma Z &= U_2^\top R U_2. \end{aligned}$$

Evidently, this is uniquely solvable for a symmetric Z so that by the inverse function theorem, \mathcal{F} is invertible in an open neighborhood of $\Delta V = 0$, and the inverse function satisfies $\overline{V} + \Delta V > 0$ in this neighborhood, by continuity. Summarizing, for any (symmetric) matrix \widehat{M} in an open neighborhood of \overline{M} there exists a positive $n \times n$ perturbation matrix

$$\widehat{V} = \overline{V} + \mathcal{F}^{-1}(\widehat{M} - \tilde{V}\tilde{V}^\top)$$

of \overline{V} , such that $\widehat{M} = \widehat{V}\widehat{V}^\top + \tilde{V}\tilde{V}^\top = \widehat{V}\widehat{V}^\top + \sum_{j=n+1}^k \mathbf{v}_j \mathbf{v}_j^\top \in \mathcal{C}_n^*$, which establishes $\text{cpr } \widehat{M} \leq k$. But we know from [18, Cor 2.5] that all matrices

$\widehat{M} \in \mathcal{C}_n^*$ which are sufficiently close to \overline{M} have $\text{cpr } \widehat{M} \geq k$, so we conclude $\widehat{M} \in \mathcal{C}_{n,k}^*$, hence \overline{M} is an inner point of $\mathcal{C}_{n,k}^*$, and the results follow. \square

5 New bounds for the cp-rank

In this section we prove that the known upper bound b_n on the cp-rank of $n \times n$ matrices can be reduced, for every $n \geq 6$. For $n = 6$ we reduce the bound further in the next section. First, we combine the idea of [17] with Theorem 2.1 to show that p_n is strictly less than b_n for every $n \geq 3$.

Theorem 5.1 *For $n \geq 2$, if $A \in \partial\mathcal{C}_n$ has $k \geq 2$ positive diagonal elements, and $M \in \mathcal{C}_n^*$ is orthogonal to A , then $\text{cpr } M \leq b_n - k + 1$.*

Proof. We may assume that $A_{ii} > 0$ for $i \in \{1, \dots, k\}$. Let

$$\mathcal{L} = \left\{ B \in \mathcal{S}_n : \mathbf{e}_i^\top B \mathbf{e}_i = 0, \text{ all } i \in \{1, \dots, k\} \right\}.$$

Then $\{\mathbf{v}\mathbf{v}^\top : \mathbf{v} \in \mathbb{R}_+^n \text{ and } \mathbf{v}^\top A \mathbf{v} = 0\} \subseteq \mathcal{L}$ by Theorem 2.1. The subspace \mathcal{L} is isomorphic to the solution space of the homogenous system of k equations in variables b_{ij} , $1 \leq i \leq j \leq n$,

$$A_{ii}b_{ii} + \sum_{j < i} A_{ij}b_{ji} + \sum_{i < j} A_{ij}b_{ij} = 0, \quad i \in \{1, \dots, k\}.$$

Since the diagonal matrix with A_{ii} , $i = 1, \dots, k$, on the diagonal is a submatrix of the coefficients matrix, the rank of the coefficients matrix is k . Thus $\dim \mathcal{L} = \binom{n+1}{2} - k$. Next suppose $M \in \mathcal{C}_n^*$ is orthogonal to $A \in \partial\mathcal{C}_n$. Then $M \in \text{conv}\{\mathbf{v}\mathbf{v}^\top : \mathbf{v} \in \mathbb{R}_+^n \text{ and } \mathbf{v}^\top A \mathbf{v} = 0\}$ which is a convex cone contained in \mathcal{L} , and by Caratheodory's theorem $\text{cpr } M \leq \dim \mathcal{L} = \binom{n+1}{2} - k$. \square

Thus for certain completely positive matrices on $\partial\mathcal{C}_n^*$ we get the following bound on the cp-rank:

Corollary 5.1 *For $n \geq 5$, if $A \in \partial\mathcal{C}_n \setminus \mathcal{N}_n$, and $M \in \mathcal{C}_n^*$ is orthogonal to A , then $\text{cpr } M \leq b_n - 4$.*

Proof. We may assume $A \in \text{ext } \mathcal{C}_n$. If A is positive-semidefinite it follows from orthogonality and $M \succeq 0$ that $\text{rank}(M) \leq n - 1$ and thus, by (3), $\text{cpr}(M) \leq b_{n-1} \leq b_n - 4$. We now assume that A is indefinite. By Lemma 3.1, A has at least 5 positive diagonal entries, since otherwise we would have $A = S \oplus O$, where S is a copositive matrix of order at most 4, so that $S \in \mathcal{P}_4 + \mathcal{N}_4$, therefore $A \in \mathcal{P}_n + \mathcal{N}_n$, and by extremality, A would

be either positive-semidefinite or nonnegative. \square

It is beneficial to introduce a cp-rank bound for positive matrices at the boundary of \mathcal{C}_n^* : Let $p_n^* := \max \left\{ \text{cpr } M : M \in \partial\mathcal{C}_n^*, \min_{i,j} M_{ij} > 0 \right\}$.

Theorem 5.2 *For $n \geq 2$, there exists a positive matrix $M \in \partial\mathcal{C}_n^* \setminus \partial\mathcal{N}_n$ such that*

$$p_n \leq \text{cpr } M + 1.$$

Hence we get

$$p_n^* \leq p_n \leq p_n^* + 1; \quad (6)$$

the right inequality is an equality for $n \in \{2, 3\}$ whereas the left inequality is an equality for $n \in \{4, 5\}$.

Proof. Let $\bar{M} \in [\mathcal{C}_n^*]^\circ$ be a matrix such that $\text{cpr } \bar{M} = p_n$ [18, Cor.2.5]. Let $\delta > 0$ be such that $M = \bar{M} - \delta \mathbf{e}_n \mathbf{e}_n^\top \in \partial\mathcal{C}_n^*$. Clearly, $p_n = \text{cpr } \bar{M} \leq \text{cpr } M + 1$. Since M has positive off-diagonal entries in the last row and it is positive-semidefinite, we have $M_{nn} > 0$ and thus M is positive, so that $\text{cpr } M \leq p_n^*$. Hence $p_n^* \leq p_n \leq p_n^* + 1$. The last assertions follow from $b_2 = 2 = p_3 - 1$ and from the fact that there are singular positive matrices $M \in \partial\mathcal{C}_n^*$ with $\text{cpr } M = p_n$ for $n \in \{4, 5\}$ [18, Rem.2.1, Cor.4.1]. \square

Remark 5.1 *For $n \leq 4$, the matrix M in Theorem 5.2 is necessarily singular. Thus for $n = 2$, $\text{rank } M = 1$ and $\text{cpr } M = 1$, which yields $p_2 \leq 2$, a tight bound. If $n \in \{3, 4\}$ then $\text{rank } M = n - 1$, and thus $\text{cpr } M \leq b_{n-1}$, and $p_n \leq \binom{n}{2}$. For $n = 3$ this gives $p_3 \leq 3$, which is also a tight bound. But for $n = 4$ this yields $p_4 \leq 6$, which is not tight. For $n = 5$, it turns out that though $p_5 = p_5^*$ is attained at a singular matrix [18, Cor.4.1], we have $p_5 = 6 < \binom{5}{2} = 10$. Still, for $n \geq 6$ we get an improvement of the known bound $p_n \leq b_n$, and for $n = 6$ we will improve it further below.*

By the above, for the first time we have a proof that b_n is not a tight upper bound on the cp-rank of completely positive matrices of any order $n \geq 5$. More precisely:

Corollary 5.2 *For $n \geq 5$, we have*

$$p_n^* \leq b_n - 4 \quad \text{and} \quad p_n \leq b_n - 3.$$

Proof. Let $M \in \partial\mathcal{C}_n^* \setminus \partial\mathcal{N}_n$ be a positive matrix with $\text{cpr } M = p_n^*$. M is orthogonal to a matrix $A \in \text{ext } \mathcal{C}_n$. As M is positive, $A \notin \mathcal{N}_n$. By Corollary 5.1, $\text{cpr } M \leq b_n - 4$, and $p_n \leq b_n - 3$ by Theorem 5.2. \square

Remark 5.2 For $n = 6$ this bound is $p_6 \leq 17$, but may be slightly improved. This case is studied in Section 6.

Beforehand we note a further result valid for arbitrary order.

Theorem 5.3 If $M \in \mathcal{C}_n^*$ has a zero entry, i.e, $M \in \partial\mathcal{N}_n$, then

$$\text{cpr } M \leq 2p_{n-1}.$$

Proof. We may and do suppose that $M_{1n} = 0$. Let $M = \sum_{i=1}^p \mathbf{w}_i \mathbf{w}_i^\top$ be a cp-decomposition of M . Define $\Omega_1 := \{i \in \{1, \dots, p\} : 1 \in \sigma(\mathbf{w}_i)\}$ and $\Omega_2 := \{1, \dots, p\} \setminus \Omega_1$, as well as $M_j := \sum_{i \in \Omega_j} \mathbf{w}_i \mathbf{w}_i^\top$, for $j = 1, 2$. Then $M_1 = M'_1 \oplus 0$ and $M_2 = 0 \oplus M'_2$, where M'_1, M'_2 are matrices in \mathcal{C}_{n-1}^* . The result follows from $\text{cpr } M = \text{cpr } (M_1 + M_2) \leq \text{cpr } M_1 + \text{cpr } M_2 = \text{cpr } M'_1 + \text{cpr } M'_2 \leq 2p_{n-1}$. \square

Remark 5.3 Note that for all $n \geq 6$, we have $2d_{n-1} \leq b_n - 3$, the bound from Corollary 5.2. However, compared with the upper bound from Theorem 5.1, we have $2p_{n-1} \geq 2d_{n-1} > b_n - k + 1$, whenever $k > \frac{n}{2}$, so that Theorem 5.3 is interesting only for small k .

6 Cp-rank of matrices of order six

In this section we improve the upper bound on the cp-rank of completely positive matrices of order 6. First we consider matrices in $\partial\mathcal{C}_6^*$ which are orthogonal to $S \oplus 0$, where $S \in \text{ext } \mathcal{C}_5$ is either in the orbit of the 5×5 Horn matrix H or a Hildebrand matrix. Below, we use the symbol “ \boxplus ” to denote the sum modulo 5 of two elements in $\{1, 2, 3, 4, 5\}$.

Proposition 6.1 Let S be either in the orbit of the 5×5 Horn matrix H or a Hildebrand matrix. Suppose that $M \in \mathcal{C}_6^*$ is orthogonal to $S \oplus 0$. Then $\text{cpr } M \leq 15$.

Proof. If $M = VV^\top$, $V \geq 0$, then each column of V is a nonnegative linear combination of three vectors, \mathbf{e}_6 , $\mathbf{e}_i + \mathbf{e}_{i \boxplus 1}$ and $\mathbf{e}_{i \boxplus 1} + \mathbf{e}_{i \boxplus 2}$ [18, Thm.4.4]. Let

$$W = [\mathbf{e}_1 + \mathbf{e}_2 | \mathbf{e}_2 + \mathbf{e}_3 | \mathbf{e}_3 + \mathbf{e}_4 | \mathbf{e}_4 + \mathbf{e}_5 | \mathbf{e}_5 + \mathbf{e}_1 | \mathbf{e}_6].$$

Then $V = WX$ where each column of X has support of at most 3 elements, contained in a set of the form $\{i, i \boxplus 1, 6\}$. For each $1 \leq i \leq 5$, let X_i consist of the columns of X whose support is contained in $\{i, i \boxplus 1, 6\}$. Then, up to permutations of rows and columns, $X_i X_i^\top = Y_i \oplus 0$ with $Y_i \in \mathcal{C}_3^*$ so that

$$\text{cpr } X_i X_i^\top = \text{cpr } Y_i \leq p_3 = 3.$$

Therefore $\text{cpr } XX^\top = \text{cpr } \sum_{i=1}^5 X_i X_i^\top \leq \sum_{i=1}^5 \text{cpr } X_i X_i^\top \leq 15$. \square

Theorem 6.1 $p_6 \leq 15$.

Proof. By [18, Thm.3.4], we know $p_6 = \text{cpr } M$ for some $M \in \partial\mathcal{C}_6^* \setminus \partial\mathcal{P}_6$. Moreover, if M had a zero entry, we get from Theorem 5.3 that $\text{cpr } M \leq 2p_5 = 12$. Suppose now that $M \in \partial\mathcal{C}_6^* \setminus (\partial\mathcal{P}_6 \cup \partial\mathcal{N}_6)$. Then Corollary 3.1 gives $\text{rank } A \geq 3$ for all $A \in \text{ext } \mathcal{C}_6 \cap M^\perp \setminus \{O\}$, and at least one such A exists as $M \in \partial\mathcal{C}_6^*$. Now either all diagonal elements of A are positive, in which case by Theorem 5.1 $\text{cpr } M \leq b_6 - 5 = 15$, or A has at least one zero on the diagonal. By Lemma 3.1, $A = S \oplus O$ with $S \in \text{ext } \mathcal{C}_5$. Since $\text{rank } S = \text{rank } A \geq 3$, we conclude that S is either in the orbit of H or a Hildebrand matrix. Then Proposition 6.1 gives $\text{cpr } M \leq 15$, and the claim is proved. \square

We thus cut the bracket for p_6 in about half, since $b_6 = 20$ and $d_6 = 9$. The same argument could be used also for $n \in \{7, 8\}$, but it would not further improve upon the bounds yielded already by the general improvement in Corollary 5.2.

References

- [1] Francesco Barioli and Abraham Berman. The maximal cp-rank of rank k completely positive matrices. *Linear Algebra Appl.*, 363:17–33, 2003.
- [2] Abraham Berman and Naomi Shaked-Monderer. Remarks on completely positive matrices. *Linear and Multilinear Algebra*, 44:149–163, 1998.
- [3] Abraham Berman and Naomi Shaked-Monderer. *Completely positive matrices*. World Scientific Publishing Co. Inc., River Edge, NJ, 2003.
- [4] Immanuel M. Bomze. Copositive optimization – recent developments and applications. *Europ. J. Oper. Research*, 216:509–520, 2012.
- [5] Immanuel M. Bomze, Werner Schachinger, and Gabriele Uchida. Think co(mpletely)positive ! – matrix properties, examples and a clustered bibliography on copositive optimization. *J. Global Optim.*, 52:423–445, 2012.
- [6] Samuel Burer. Copositive programming. In Miguel F. Anjos and Jean Bernard Lasserre, editors, *Handbook of Semidefinite, Cone and Polynomial Optimization: Theory, Algorithms, Software and Applications*, International Series in Operations Research and Management Science, pages 201–218. Springer, New York, 2012.
- [7] Palahenedi Hewage Diananda. On non-negative forms in real variables some or all of which are non-negative. *Proc. Cambridge Philos. Soc.*, 58:17–25, 1962.

- [8] Peter J.C. Dickinson. An improved characterisation of the interior of the completely positive cone. *Electron. J. Linear Algebra*, 20:723–729, 2010.
- [9] John H. Drew and Charles R. Johnson. The no long odd cycle theorem for completely positive matrices. In *Random discrete structures*, IMA Vol. Math. Appl. 76, Springer, New York, 1996, pages 103–115.
- [10] John H. Drew, Charles R. Johnson, and Raphael Loewy. Completely positive matrices associated with M -matrices. *Linear and Multilinear Algebra*, 37:303–310, 1994.
- [11] Mirjam Dür. Copositive programming — a survey. In Moritz Diehl, Francois Glineur, Elias Jarlebring, and Wim Michiels, editors, *Recent Advances in Optimization and its Applications in Engineering*, pages 3–20. Springer, Berlin Heidelberg New York, 2010.
- [12] Mirjam Dür and Georg Still. Interior points of the completely positive cone. *Electron. J. Linear Algebra*, 17:48–53, 2008.
- [13] Marshall Hall, Jr. and Morris Newman. Copositive and completely positive quadratic forms. *Proc. Cambridge Philos. Soc.*, 59:329–339, 1963.
- [14] Roland Hildebrand. The extremal rays of the 5×5 copositive cone. *Linear Algebra and its Applications*, 437:1538–1547, 2012.
- [15] Mohammed Kaykobad. On nonnegative factorization of matrices. *Linear Algebra Appl.*, 96:27–33, 1987.
- [16] Raphael Loewy and Bit-Shun Tam. CP rank of completely positive matrices of order 5. *Linear Algebra Appl.*, 363:161–176, 2003.
- [17] Naomi Shaked-Monderer. A note on upper bounds on the cp-rank. *Linear Algebra Appl.*, 431:2407–2413, 2009.
- [18] Naomi Shaked-Monderer, Immanuel M. Bomze, Florian Jarre, and Werner Schachinger. On the cp-rank and minimal cp factorizations of a completely positive matrix. *SIAM J. Matrix Anal. Appl.*, to appear, 2013.